

and other penalties.

\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 10:10:21 ON 24 JUN 2009

|                      |            |         |
|----------------------|------------|---------|
| => file reg          |            |         |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL   |
|                      | ENTRY      | SESSION |
| FULL ESTIMATED COST  | 0.22       | 0.22    |

FILE 'REGISTRY' ENTERED AT 10:10:40 ON 24 JUN 2009  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file  
 provided by InfoChem.

STRUCTURE FILE UPDATES: 22 JUN 2009 HIGHEST RN 1159446-15-7  
 DICTIONARY FILE UPDATES: 22 JUN 2009 HIGHEST RN 1159446-15-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

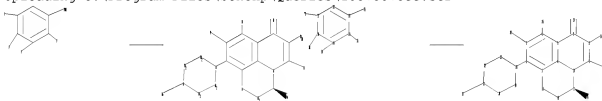
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
 predicted properties as well as tags indicating availability of  
 experimental property data in the original document. For information  
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>  
 Uploading C:\Program Files\Stnexp\Queries\10578078cc.str



chain nodes :  
 14 15 16 17 24 25 26 35 36 37 38 39  
 ring nodes :

```

1  2  3  4  5  6  7  8  9 10 11 12 13 18 19 20 21 22 23 29 30 31 32
33 34
chain bonds :
2-18  3-24  4-26  7-14  8-15  9-25 11-16 17-21 29-39 30-38 31-37 33-35 34-36

ring bonds :
1-2  1-6  1-13  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10 10-11 11-12 12-13
18-19 18-23 19-20 20-21 21-22 22-23 29-30 29-34 30-31 31-32 32-33 33-34
exact/norm bonds :
1-13  2-18  5-7  6-10  7-8  7-14  8-9  9-10 10-11 11-12 12-13 18-19 18-23
19-20 20-21 21-22 22-23
exact bonds :
3-24  4-26  8-15  9-25 11-16 17-21 29-39 30-38 31-37 33-35 34-36
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  29-30 29-34 30-31 31-32 32-33 33-34

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 29:CLASS
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:CLASS 36:CLASS 37:CLASS 38:CLASS
39:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 29

```

Stereo Bonds:

16-11 (Single Wedge).

Stereo Chiral Centers:

11 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 11

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.48

0.70

FILE 'CASREACT' ENTERED AT 10:11:11 ON 24 JUN 2009  
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FILE CONTENT:1840 - 21 Jun 2009 VOL 150 ISS 26

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 16.5 million reactions
*
*****
```

CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l1

```
SAMPLE SEARCH INITIATED 10:11:16 FILE 'CASREACT'
SCREENING COMPLETE -      0 REACTIONS TO VERIFY FROM      0 DOCUMENTS

100.0% DONE      0 VERIFIED      0 HIT RXNS      0 DOCS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH  **COMPLETE**
PROJECTED VERIFICATIONS:  0 TO      0
PROJECTED ANSWERS:       0 TO      0
```

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s l1 sss full

```
FULL SEARCH INITIATED 10:11:23 FILE 'CASREACT'
SCREENING COMPLETE -     115 REACTIONS TO VERIFY FROM     10 DOCUMENTS

100.0% DONE     115 VERIFIED      8 HIT RXNS      3 DOCS
SEARCH TIME: 00.00.02
```

L3 3 SEA SSS FUL L1 ( 8 REACTIONS)

=> d ibib abs fhlt tot

13 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
 ACCESSION NUMBER: 14448205 CASREACT  
 TITLE: Synthetic process for the preparation of levofloxacin hemihydrate from levofloxacin  
 INVENTOR(S): Rao, Javaluri Ramobhavi Dalveedi, Bhikshakshi Bhar; Neem (Kandlu, Ramulu Babu, Arundha)  
 Transalabachari,  
 PATENT ASSIGNER(S): Newland Laboratories Ltd., India  
 SOURCE: PCT Int. Appl., 31 pp.  
 COUNTRY: PTOCD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACQ. ILM. COUNT: 1  
 PATENT INFORMATION: 1

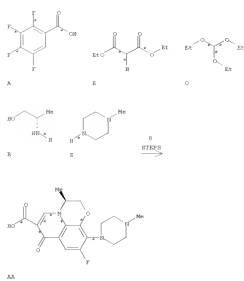
| PATENT NO.   | KIND DATE   | APPLICATION NO. | DATE     |
|--|-------------|-----------------|----------|
| NO 2004040899  | AL 20040408 | NO 2004-10142   | 20041109 |
| Wt, Ar, AG, Al, AM, AT, AR, AU, BA, BB, BE, BM, BT, BR, CA, CB, CH, CO, CU, CY, DE, DK, DM, DO, DR, ES, EU, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KS, LG, LU, LV, LY, MC, MD, ME, MG, MN, MU, MY, NZ, OM, PA, PE, PG, PH, PL, PT, PY, RE, RU, SA, SD, SG, SI, SK, SL, SM, SN, SR, ST, SV, SW, TH, TR, TT, UA, US, UG, UZ, VC, VN, YD, ZA, ZM, ZW |             |                 |          |
| IMP AT, AU, CA, CH, CO, CU, DE, DK, DM, DO, DR, ES, EU, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KS, LG, LU, LV, LY, MC, MD, ME, MG, MN, MU, MY, NZ, OM, PA, PE, PG, PH, PL, PT, PY, RE, RU, SA, SD, SG, SI, SK, SL, SM, SN, SR, ST, SV, SW, TH, TR, TT, UA, US, UG, UZ, VC, VN, YD, ZA, ZM, ZW   |             |                 |          |
| US 20070248318   | AL 20071018 | US 2004-578078  | 20040811 |
| US 5693637   | US 20070725 | EP 2004-806742  | 20041109 |
| At, Ar, AG, Al, AM, AT, AR, AU, BA, BB, BE, BM, BT, BR, CA, CB, CH, CO, CU, CY, DE, DK, DM, DO, DR, ES, EU, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KS, LG, LU, LV, LY, MC, MD, ME, MG, MN, MU, MY, NZ, OM, PA, PE, PG, PH, PL, PT, PY, RE, RU, SA, SD, SG, SI, SK, SL, SM, SN, SR, ST, SV, SW, TH, TR, TT, UA, US, UG, UZ, VC, VN, YD, ZA, ZM, ZW |             |                 |          |

AB A process for preparation of Levofloxacin hemihydrate, having single isomer (S-isomer)

impurity not more than 0.1% and free from particulate matter and from the other enantiomer (R-form), is described which comprises: dissolving levofloxacin tech. grade in an aqueous alkaline solution, treating the solution with activated carbon at room temperature; removing the undissolved particulate matter by filtration; bringing the pH of the aqueous alkaline levofloxacin solution to neutral using dilute mineral acid; removing the precipitated particulate matter; by filtration; acidifying the resulting solution; treating the acidified solution with activated carbon at room temperature; filtering the undissolved particulate matter by filtration; neutralizing the acidic solution; filtering again to remove any particulate matter present; and extracting the resulting product with a chlorinated solvent (e.g., DCE/CH<sub>2</sub>Cl<sub>2</sub>) and concentrating under vacuum

13 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
 using aq. THF or an aprotic with other org. solvents to get highly pure levofloxacin hemihydrate having a single individual impurity which is <0.1% and is free from particulate matter and from the other enantiomer (R-form).

KK(14) OF 36 COMPOSED OF KK(1), KK(12), KK(13), KK(14), KK(15), KK(16), KK(17), KK(18)  
 KK(14) A + E + O + R + Z ==> AA



KK(1) RCT A 1401-31-E  
 RCT C 7719-09-7 SOC12

13 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
 PRO 3 94695-49-4  
 SOL 68-12-2 H<sub>2</sub>O  
 CON SUBSTAGE(1) room temperature -> 90 deg C  
 SUBSTAGE(2) 4 - 8 hours

KK(2) RCT E 105-15-3

STAGE(1)  
 SOL 64-17-5 EtOH, 100-80-3 PhMe  
 CON 20 minutes, room temperature

STAGE(2)  
 RCT 3 9439-95-4 Mg  
 CAT 67-66-3 CHCl<sub>3</sub>  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 20 minutes, room temperature  
 SUBSTAGE(3) 3 - 4 hours, 70 - 90 deg C  
 SUBSTAGE(4) 30 minutes, 70 - 90 deg C  
 SUBSTAGE(5) 90 deg C -> 55 deg C

STAGE(3)  
 RCT 3 94695-49-4  
 SOL 100-80-3 THF, 100-80-3 PhMe  
 CON SUBSTAGE(2) 30 - 35 deg C  
 SUBSTAGE(3) 35 deg C -> 5 deg C  
 SUBSTAGE(4) - 2 hours, 0 - 5 deg C  
 SUBSTAGE(5) 30 minutes, 70 - 90 deg C  
 SUBSTAGE(6) 5 deg C -> 25 deg C  
 SUBSTAGE(7) 30 minutes, 20 - 25 deg C

PRO 3 94695-49-5

KK(3) RCT F 94695-49-9  
 RCT W 104135-4-7  
 PRO L 94695-50-3  
 SOL 7732-19-5 MeOH  
 CON 3 hours, 80 - 90 deg C

KK(4) RCT L 94695-50-9, O 122-51-0  
 PRO P 94714-58-0  
 SOL 120-21-7 MeOH  
 CON SUBSTAGE(1) room temperature -> 125 deg C  
 SUBSTAGE(2) 4 hours, 120 - 115 deg C

KK(5) RCT F 94714-58-6, R 2749-11-3  
 PRO S 130148-02-2  
 RCT 78-09-3 CHCl<sub>3</sub>  
 CON SUBSTAGE(1) 20 - 35 deg C  
 SUBSTAGE(2) 35 deg C -> 5 deg C  
 SUBSTAGE(3) - 2 hours, 0 - 5 deg C  
 SUBSTAGE(4) 5 deg C -> 35 deg C  
 SUBSTAGE(5) 2 hours, 30 - 35 deg C

KK(6) RCT S 130148-02-2  
 RCT V 954-09-7 HCOOH  
 PRO U 100939-34-8  
 SOL 68-12-2 H<sub>2</sub>O

13 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
 CON SUBSTAGE(1) 120 deg C  
 SUBSTAGE(2) 2 hours, 120 deg C  
 SUBSTAGE(3) 30 minutes

KK(7) RCT U 106939-34-8  
 RCT X 7647-81-0 HCl  
 PRO W 100994-89-8  
 SOL 7732-19-5 MeOH, 64-19-7 AcOH  
 CON SUBSTAGE(1) room temperature -> 80 deg C  
 SUBSTAGE(2) 6 hours, 75 - 80 deg C  
 SUBSTAGE(3) 80 deg C -> 20 deg C  
 SUBSTAGE(4) 1 hour, 15 - 20 deg C

KK(8) RCT W 100994-89-8, E 109-01-3  
 RCT AB 110-86-1 Pyridine  
 PRO AA 100994-85-4  
 SOL 110-86-1 Pyridine  
 CON 10 hours, room temperature -> 120 deg C

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

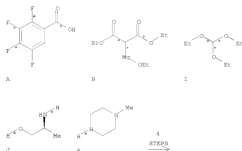
FORMAT

[illegible]

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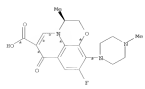
KK(10) OF 10 COMPOSED OF KK(1), KK(2), KK(3), KK(4)
KK(10)      A  +  B  +  C  +  D  +  E  ==>  S

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LJ ANSWER 2 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
RX(4) ACT R 109-01-3, G 109986-89-8  
PRO S 109986-85-4  
SOL 67-68-5 IMHO

13 ANSWER 2 OF 3 CASREACT COPYRIGHT 2002 ACS on 5TH (Continued)

5  
 YFET 028

FOI ( ) ACT A 1201-31-6

```
STAGE(1)
  BGT  D 7719-09-7 SOCI
  BGT  68-12-2 TMR
```

STAGE (2)  
RCT B 207746-86-9

STAGE(3)  
RGT E 194-15-4 TsOH

NO C 94695-50-8

FOI (2)      RCT   I 122-51-0, C 94695-50-8

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STAGE(1)
    SOL  198-24-7  Ac2O

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```
STAGE (2)
RCT J 2749-11-3
SOL 75-09-2 CH2C12
```

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STAGE(3)
  RGT  L 504-00-7 K2CO3
  SOL  60-12-2 DMF

```

67 K 106939-34-8

|       |     |                |
|-------|-----|----------------|
| FX(3) | ACT | K 106939-34-8  |
|       | RG7 | P 7647-01-0 NC |
|       | PRO | O 100986-89-8  |
|       | SOL | 64-19-7 AcOH   |

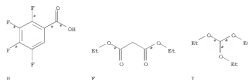
L3 ANMER 3 OF CASRAC7 COPYRIGHT 2009 ACS ON STM  
ACCESSION NUMBER: 110475530 CASRAC7  
TITLE: Process for preparation of racemic and optically  
active ofloxacin and related derivatives  
INVENTOR(S): Mitscher, Lester A.; Chu, Daniel T.  
PATENT ASSIGNEE(S): Abbott Laboratories, USA  
SOURCE: U.S., 7 pp.  
CODING: USKOW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.            | KIND | DATE              | APPLICATION NO. | DATE    |
|-----------------------|------|-------------------|-----------------|---------|
| US 4777253            | A    | 19881011          | US 1986-088532  | 1986042 |
| US 4826985            | A    | 19890502          | US 1988-216063  | 1988070 |
| PRIORITY APPL. INFO.: |      |                   | US 1986-088532  | 1986042 |
| OTHER SOURCE(S):      |      | MARKPAT 110:75530 |                 |         |
| GI                    |      |                   |                 |         |



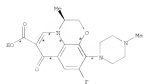
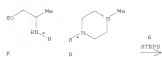
AB The title compound **1** (R1 = H, Cl-4 alkyl, FAcEt; R2 = R2(5H); R4, R5 = H, alkanoyl, alkanoylamido, substituted amino; R4(R5) = (un)substituted aliphatic heterocyclyl) (wherein the the racemate of alkanon exhibits antibacterial properties) were prepared (-)-**1** (R1 = Et; R2 = F) (preparation 1)

Quantum In pyridine was added to 1-methylpyrazole, the mixture heated to 55°C and after workup, the solid obtained was dissolved in THF and NaOH solution to give (-)-**1** (R1 = H; R2 = 4-methylpyrazinyl).

$$R_{K(86)} = H + P + T + K + R \text{ mm} > N$$


L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2009 ACS on SYN (Continued)

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2009 ACS on SYN (Continued)



B

XX(14) NCT B 1203-35-6  
PRO E 94695-48-4

XX(17) NCT E 94695-48-4, F 105-53-3  
PRO G 94695-50-5

XX(15) NCT G 94695-50-5, I 122-53-9  
PRO J 94714-58-6

XX(16) NCT J 94714-58-6, K 2749-13-3  
PRO L 130548-02-2

XX(13) NCT L 130548-02-2  
PRO P 106939-34-8  
SOL 109-99-9 THF

XX(19) NCT P 106939-34-8, R 109-01-3  
ROT Q 7732-18-5 Water  
PRO M 100906-85-4  
SOL 7732-18-5 Water

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT